Abstract:

Protein heterodimer complexes are often involved in catalysis, regulation, assembly, immunity and inhibition. This involves the formation of stable interfaces between the interacting partners. Hence, it is of interest to describe heterodimer interfaces using known structural complexes. We use a non-redundant dataset of 192 heterodimer complex structures from the protein databank (PDB) to identify interface residues and describe their interfaces using amino-acids residue property preference. Analysis of the dataset shows that the heterodimer interfaces are often abundant in polar residues. The analysis also shows the presence of two classes of interfaces in heterodimer complexes. The first class of interfaces (class A) with more polar residues than core but less than surface is known. These interfaces are more hydrophobic than surfaces, where protein-protein binding is largely hydrophobic. The second class of interfaces (class B) with more polar residues than core and surface is shown. These interfaces are more polar than surfaces, where binding is mainly polar. Thus, these findings provide insights to the understanding of protein-protein interactions.

Keywords: protein-protein interaction (PPI); heterodimer; interface; surface; core; polar abundance.